Pipes/KOH pH 6.8 (Sigma P6757), 2 mM $MgCl_2$ (VWR JT400301), and 1 mM EGTA (Sigma E3889). Solution 2 consists of 1 mM NADH (Sigma N8129), 0.2 mg/ml BSA (Sigma A7906), pyruvate kinase 7 U/ml, L-lactate dehydrogenase 10 U/ml (Sigma P0294), 100 nM KSP motor domain, 50 μg/ml microtubules, 1 mM DTT (Sigma D9779), 5 μM paclitaxel (Sigma T-7402), 10 ppm antifoam 289 (Sigma A-8436), 25 mM Pipes/KOH pH 6.8 (Sigma P6757), 2 mM MgCl2 (VWR JT4003-01), and 1 mM EGTA (Sigma E3889). Serial dilutions (8-12 two-fold dilutions) of the compound are made in a 96-well microtiter plate (Corning Costar 3695) using Solution 1. Following serial dilution each well has 50 μl of Solution 1. The reaction is started by adding 50 μl of solution 2 to each well. This may be done with a multichannel pipettor either manually or with automated liquid handling devices. The microtiter plate is then transferred to a microplate absorbance reader and multiple absorbance readings at 340 nm are taken for each well in a kinetic mode. The observed rate of change, which is proportional to the ATPase rate, is then plotted as a function of the compound concentration. For a standard IC_{50} determination the data acquired is fit by the following four parameter equation using a nonlinear fitting program (e.g., Grafit 4):

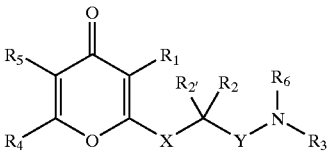
$$y = \frac{\text{Range}}{1 + \left(\frac{x}{IC_{50}}\right)^{s}} + \text{Background}$$

[0461] where y is the observed rate and x is the compound concentration.

What is claimed is:

1. A compound having the structure represented by Formula I:

(Formula I)



wherein:

X is optionally substituted alkylene, —C(O)—, or is absent;

Y is optionally substituted alkylene, —C(O)—, or is absent;

R_1 is chosen from hydrogen, optionally substituted alkyl-, optionally substituted aryl-, optionally substituted aralkyl-, optionally substituted heteroaryl-, and optionally substituted heteroaralkyl-;

R_4 and R_5 are independently chosen from hydrogen, optionally substituted alkyl, optionally substituted alkoxy, halogen, hydroxyl, nitro, cyano, optionally substituted amino, alkylsulfonyl, alkylsulfonamido, alkylsulfanyl, carboxy, carboxyalkyl, carboxamido, aminocarbonyl, optionally substituted aryl, optionally substituted aralkyl, optionally substituted heteroaralkyl and optionally substituted heteroaryl; or R_4 and R_5, taken together with the carbons to which they are bound, form an optionally substituted 5- to 7-membered non-aromatic ring;

R_2 and R_2 are independently chosen from hydrogen, optionally substituted alkyl-, optionally substituted aryl-, optionally substituted aralkyl-, optionally substituted heteroaryl-, and optionally substituted heteroaralkyl-; or R_2 and $R_{2'}$ taken together with the carbon to which they are bound, form an optionally substituted 3- to 7-membered ring;

R_3 is chosen from hydrogen, optionally substituted alkyl-, optionally substituted aryl-, optionally substituted aralkyl-, optionally substituted heteroaryl-, optionally substituted heteroaralkyl-, —C(O)—R_7, and —$S(O)_2$—R_{7a}; and R_6 is chosen from hydrogen, optionally substituted alkyl-, optionally substituted aryl-, optionally substituted aralkyl-, optionally substituted heteroaralkyl-, and optionally substituted heterocyclyl-;

or R_3 taken together with R6, and the nitrogen to which they are bound, form an optionally substituted 5- to 12-membered nitrogen-containing heterocycle, which optionally incorporates from one to two additional heteroatoms, selected from N, O, and S in the heterocycle ring;

or R_3 taken together with R_2 form an optionally substituted 5- to 12-membered nitrogen-containing heterocycle, which optionally incorporates from one to two additional heteroatoms, selected from N, O, and S in the heterocycle ring;

R_7 is chosen from hydrogen, optionally substituted alkyl-, optionally substituted aryl-, optionally substituted aralkyl-, optionally substituted heteroaryl-, optionally substituted heteroaralkyl-, —OR_8 and —NHR_{14};

R_{7a} is chosen from optionally substituted alkyl-, optionally substituted aryl-, optionally substituted aralkyl-, optionally substituted heteroaryl-, optionally substituted heteroaralkyl-, and R_{14}—NH—;

R_8 is chosen from optionally substituted alkyl-, optionally substituted aryl-, optionally substituted aralkyl-, optionally substituted heteroaryl-, and optionally substituted heteroaralkyl-; and

R_{14} is hydrogen, optionally substituted alkyl-, optionally substituted aryl-, optionally substituted aralkyl-, optionally substituted heteroaryl-, or optionally substituted heteroaralkyl- including single stereoisomers and mixtures of stereoisomers;

a pharmaceutically acceptable salt of a compound of Formula I;

a pharmaceutically acceptable solvate of a compound of Formula I;

or a pharmaceutically acceptable solvate of a pharmaceutically acceptable salt of a compound of Formula I.